

Li-ion Battery Solid Electrolyte Interface (SEI) investigation with in-situ Attenuated Total Reflection-Infrared (ATR-IR) spectroscopy

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In order to design safer, higher-energy batteries with prolonged lifetime, it is desired for us to better understand the surface reactions occurring on the electrode and generating a Solid Electrolyte Interphase (SEI). Due to the nature of SEI as an amorphous, multicomponent film, to characterize its chemical composition, it is essential to be able to detect and identify the vibrations of different organic function group. Infrared spectroscopy has been known as a widely used technique to probe the surface reaction mechanism. However, most of the results reported in previous literatures are from ex-situ measurements, thus not able to provide comprehensive information to determine the real composition of SEI, which is critical to reveal the reaction mechanism.

In present study, we developed a novel in-situ ATR-IR approach and the real time SEI formation was probed on two metal surfaces, Au and Sn. For the purpose of comparison ex-situ ATR-IR was performed on the same surfaces. Several new features were captured from in-situ spectrum, comparing with ex-situ spectrum. By peak assignment, the new product detected from in-situ test was found to be Li propionate, which dissolved into the solvent during the DMC washing procedure in ex-situ test. Significant variations in SEI components and mechanisms were captured on the two metal surfaces, despite of the same reduction condition.

In addition to the traditional components reported in ex-situ experiment, we also probed some other soluble products that could never been found with DMC washing on both Au and Sn surface. These in-situ spectrum results shed light on some unknown procedures related to the formation of the films, which might be detrimental on battery performance in one way or another.

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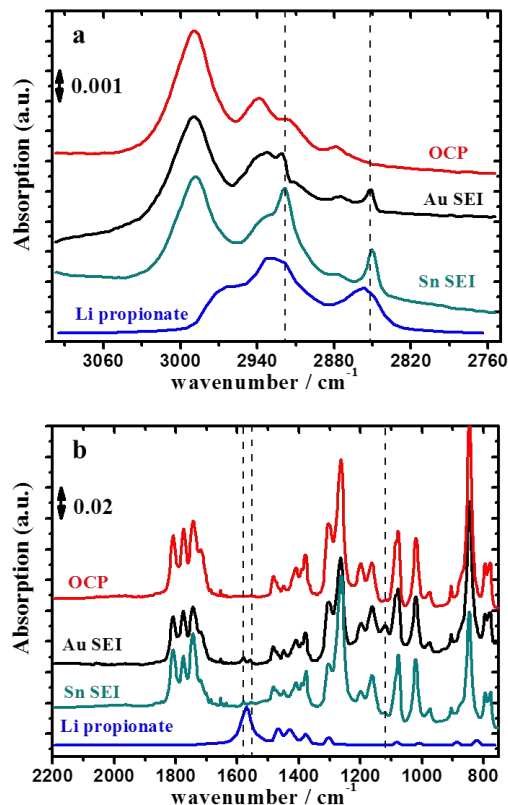


Figure 1. IR spectra obtained in the ATR mode from Au and Sn electrode after potential step from OCP to 0.1V in EC/DEC 1M LiPF₆ electrolyte. (a) C-H stretching vibration region; (b) C-O vibration region.